

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
 Data File : BM049805.D
 Acq On : 03 Apr 2025 14:37
 Operator : RC/JU
 Sample : Q1693-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WCS-TP-2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	3	5	14	rVB	135291	175659	1.09%	0.223%
2	4.904	320	326	338	rBV	1013476	1377217	8.54%	1.751%
3	5.369	399	405	416	rBV	5424085	7421548	46.02%	9.436%
4	5.981	504	509	515	rVB	164687	236797	1.47%	0.301%
5	6.957	667	675	691	rBV	5127260	7738907	47.98%	9.840%
6	7.786	809	816	823	rVB	1070545	1647605	10.22%	2.095%
7	8.939	999	1012	1022	rBV	2935906	4622563	28.66%	5.877%
8	10.580	1281	1291	1297	rBV	1262715	2051940	12.72%	2.609%
9	13.051	1703	1711	1722	rBV	7686461	10799800	66.96%	13.731%
10	14.145	1891	1897	1903	rBV	112910	174865	1.08%	0.222%
11	14.427	1936	1945	1952	rBV	1864994	2700938	16.75%	3.434%
12	15.786	2170	2176	2184	rBV	582351	763307	4.73%	0.971%
13	15.915	2191	2198	2216	rBV	6632162	8802985	54.58%	11.193%
14	17.168	2405	2411	2416	rBV	2310670	3049330	18.91%	3.877%
15	18.074	2559	2565	2572	rBV	556678	872865	5.41%	1.110%
16	19.221	2756	2760	2767	rVB	272703	367902	2.28%	0.468%
17	19.350	2778	2782	2784	rBV	223105	277992	1.72%	0.353%
18	19.586	2818	2822	2825	rBV	291676	353135	2.19%	0.449%
19	19.792	2852	2857	2869	rVB	14331992	16128294	100.00%	20.506%
20	19.909	2873	2877	2886	rBV7	79234	171845	1.07%	0.218%
21	20.780	3022	3025	3029	rBV4	165967	216518	1.34%	0.275%
22	21.091	3074	3078	3088	rBV2	340163	588557	3.65%	0.748%
23	21.403	3124	3131	3136	rBV	2591902	4027321	24.97%	5.121%
24	24.256	3611	3616	3628	rVB	324470	763144	4.73%	0.970%
25	24.403	3633	3641	3649	rBV	1393816	3319631	20.58%	4.221%

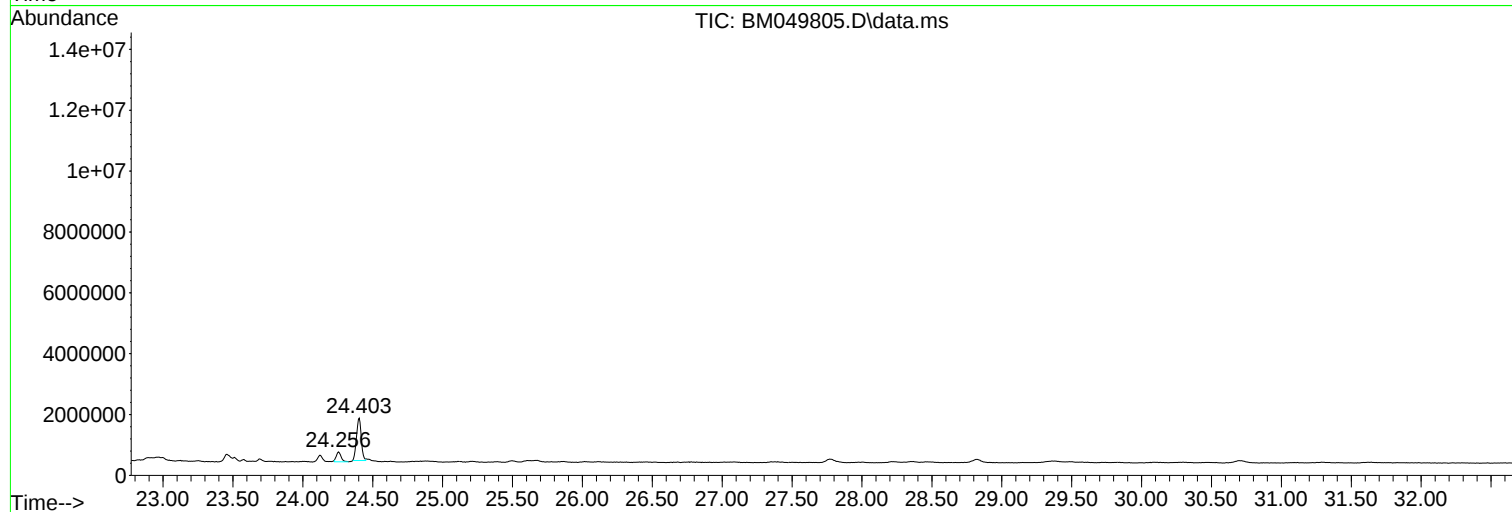
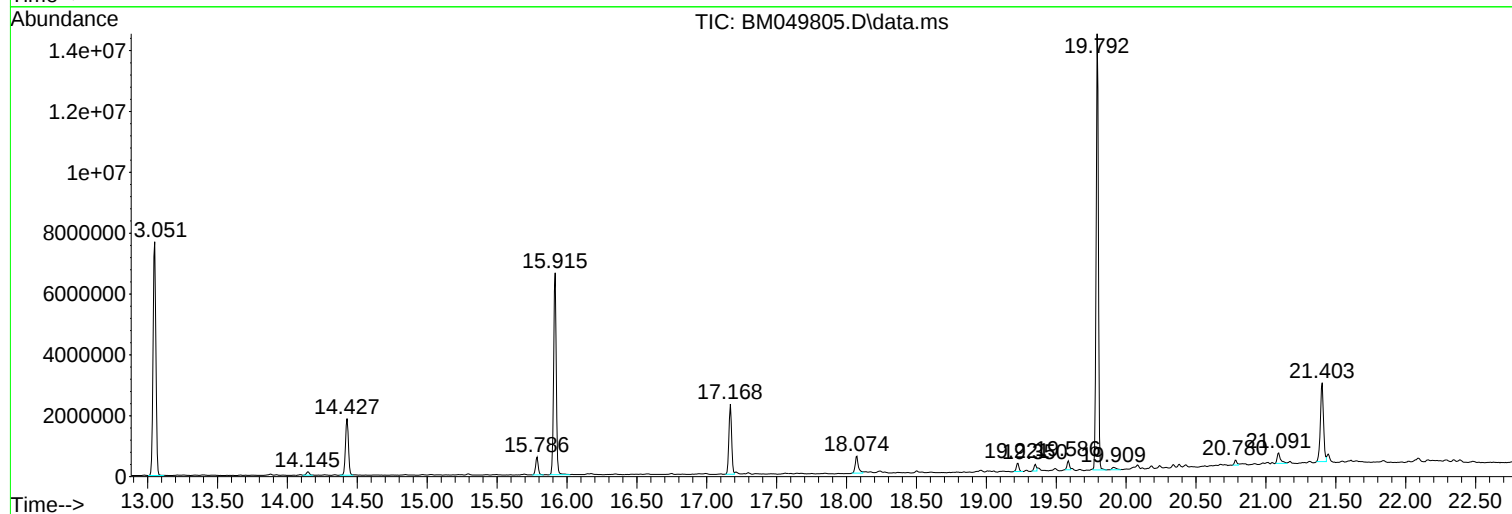
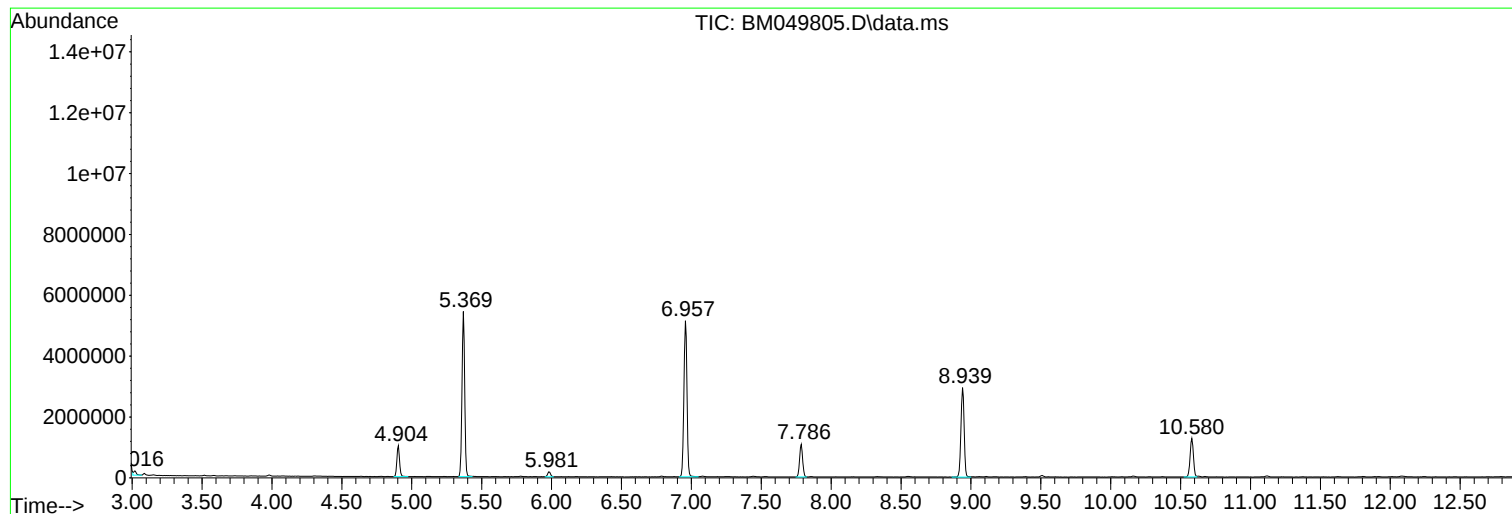
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ClientSampleId :
WCS-TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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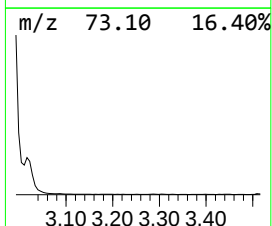
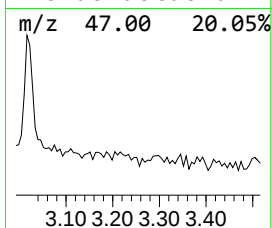
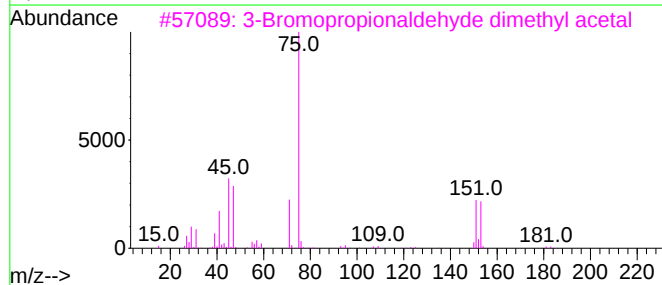
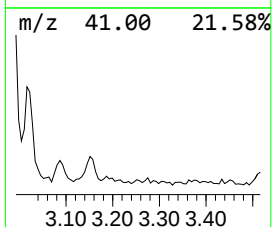
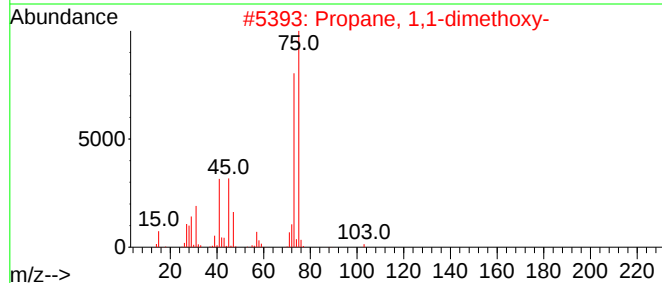
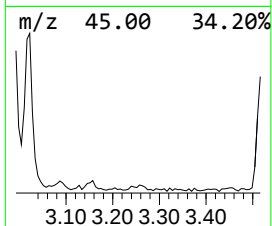
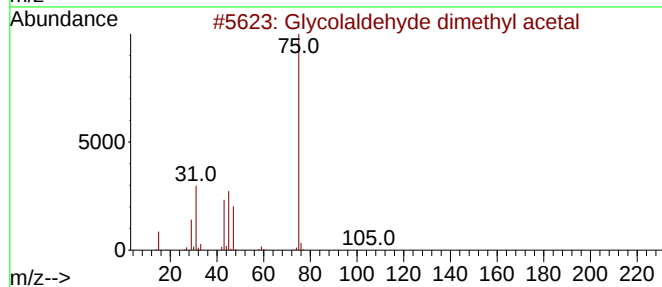
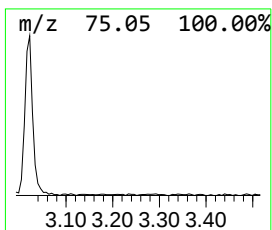
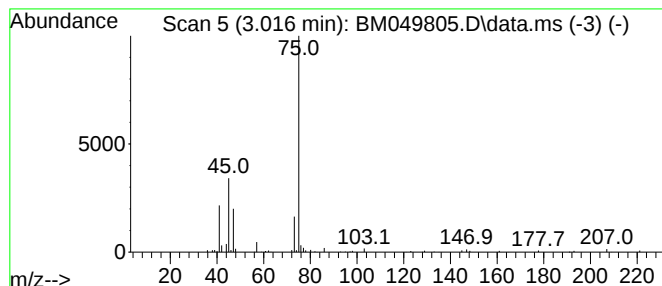
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Glycolaldehyde dimethyl acetal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.016	2.13 ng	175659	1,4-Dichlorobenzene-d4	7.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	64
2			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
3			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	39
4			2-Azabutane, N-amidino-4,4-dimet...	161	C6H15N3O2	052737-41-4	9
5			Ethane, 1,1,2,2-tetramethoxy-	150	C6H14O4	002517-44-4	9



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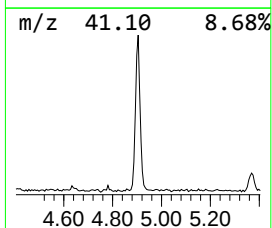
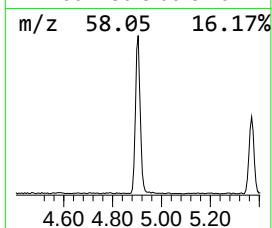
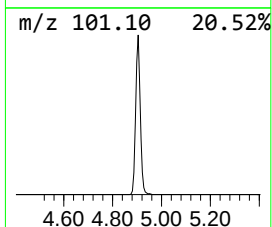
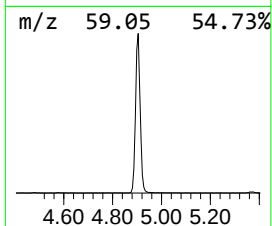
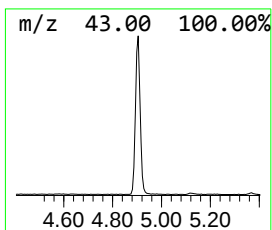
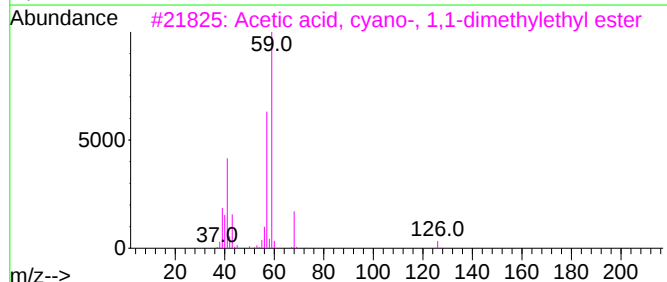
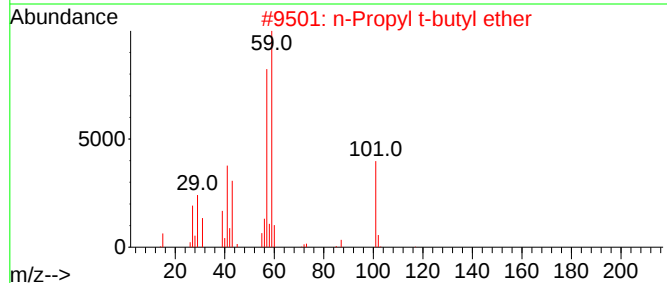
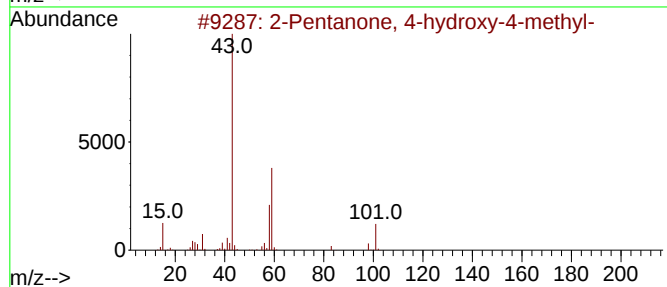
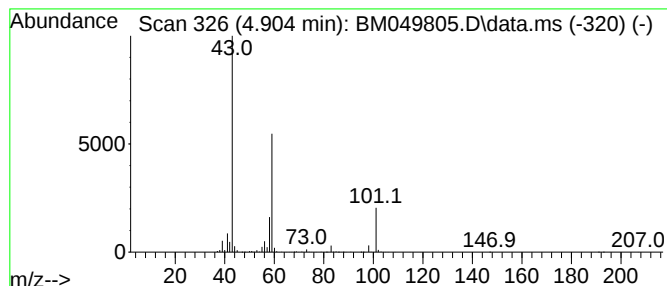
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	16.72 ng	1377220	1,4-Dichlorobenzene-d4	7.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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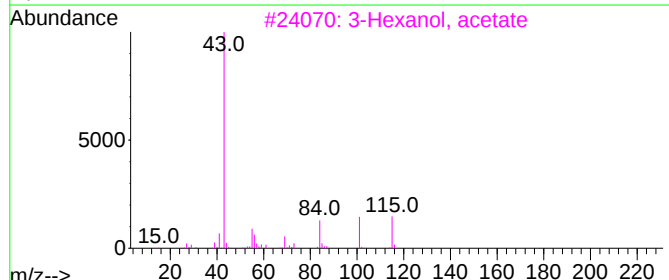
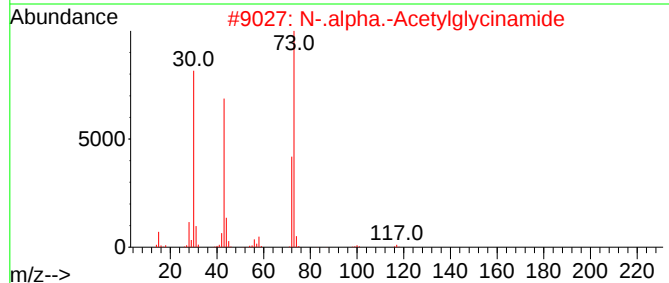
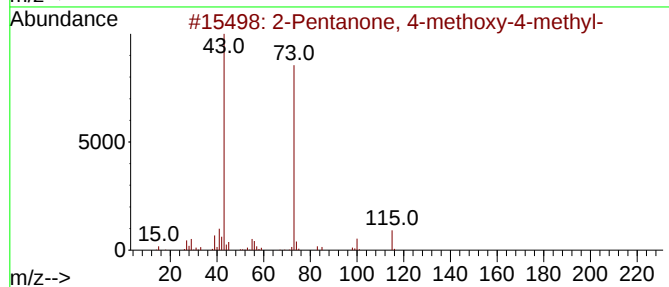
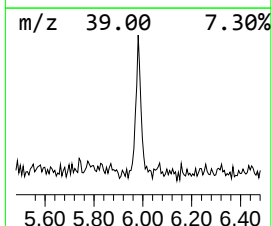
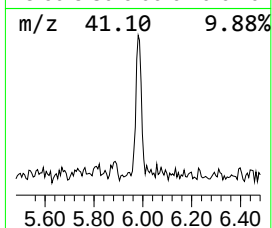
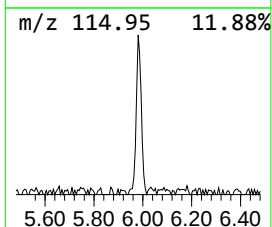
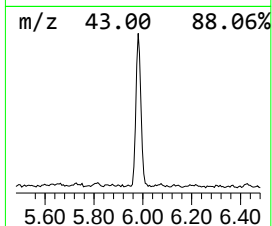
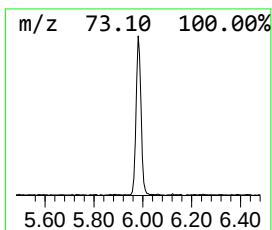
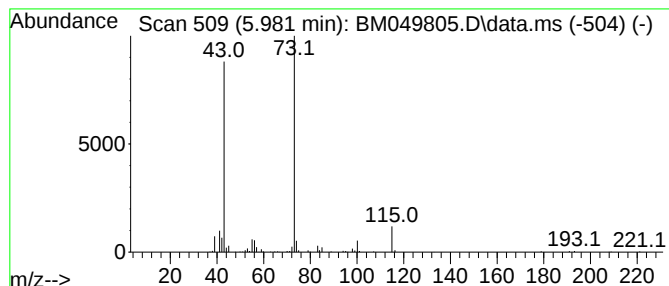
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	2.87 ng	236797	1,4-Dichlorobenzene-d4	7.786

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40
3		3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16
5		N-Ethylformamide	73	C3H7NO	000627-45-2	16



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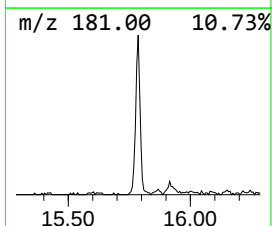
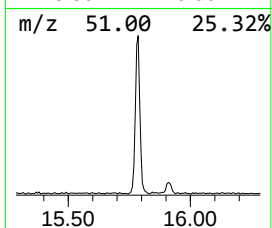
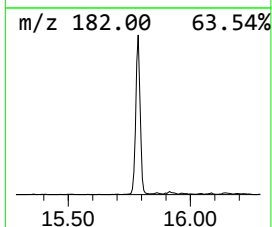
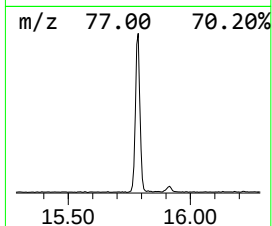
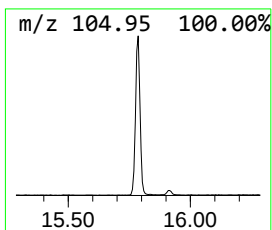
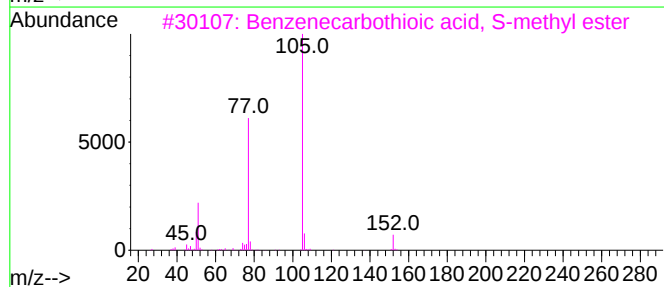
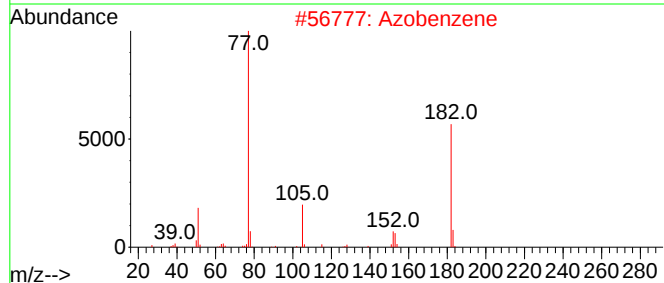
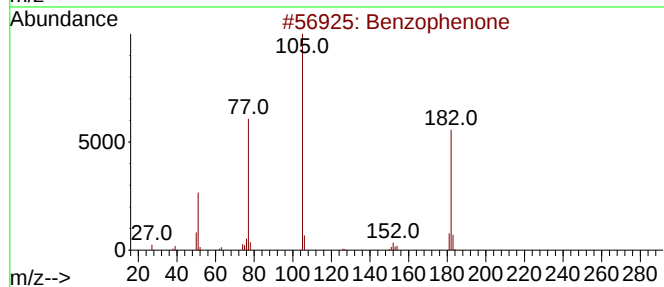
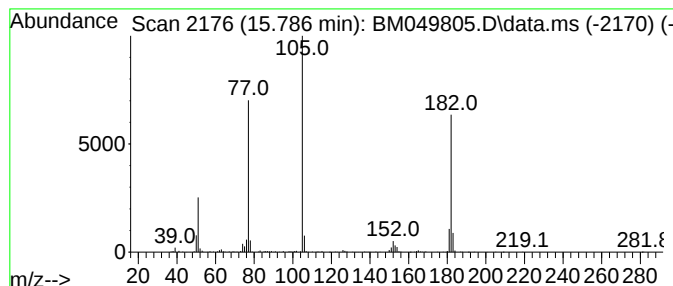
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Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	5.65 ng	763307	Acenaphthene-d10	14.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	49
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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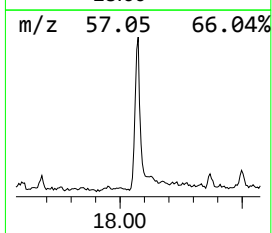
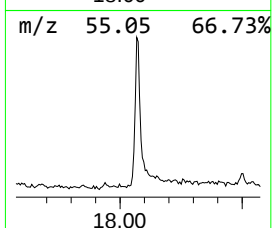
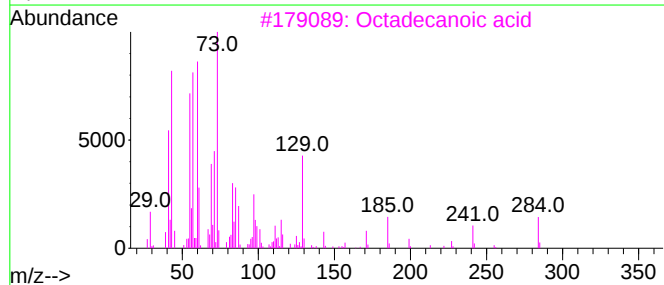
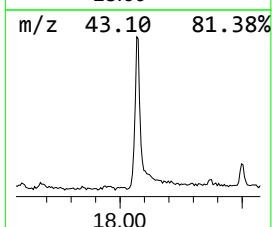
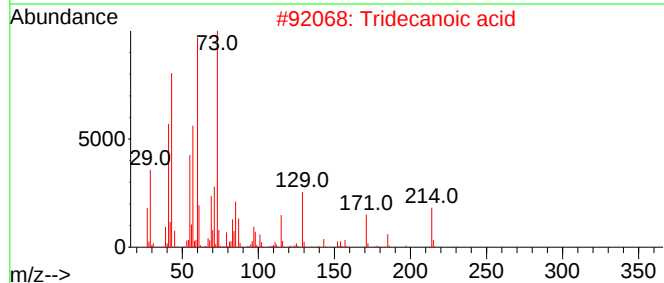
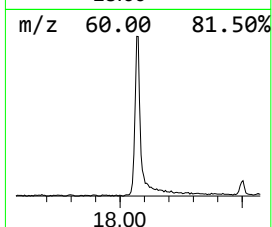
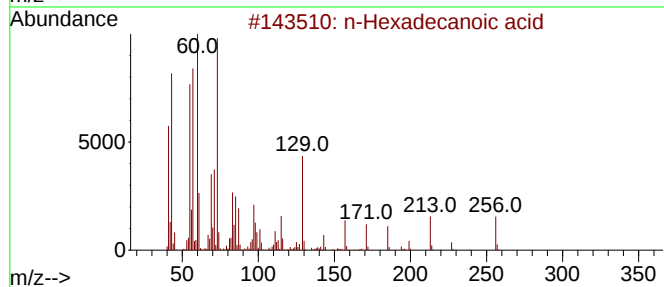
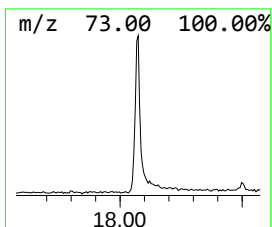
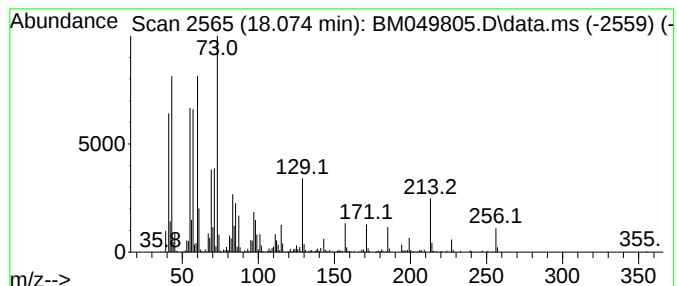
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	5.72 ng	872865	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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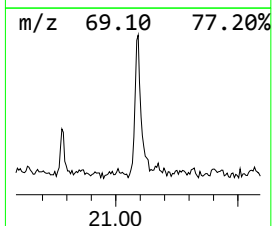
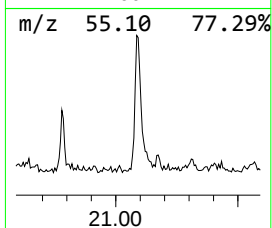
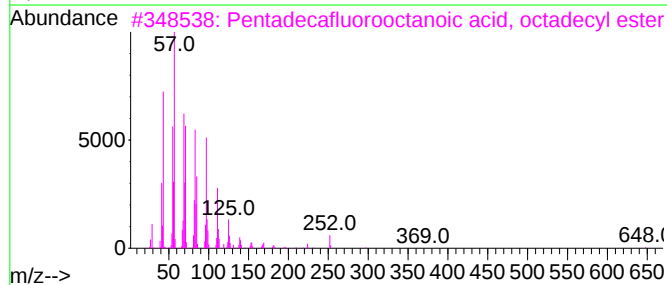
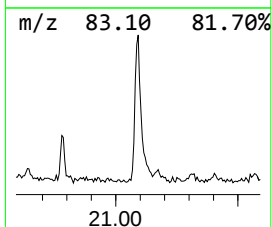
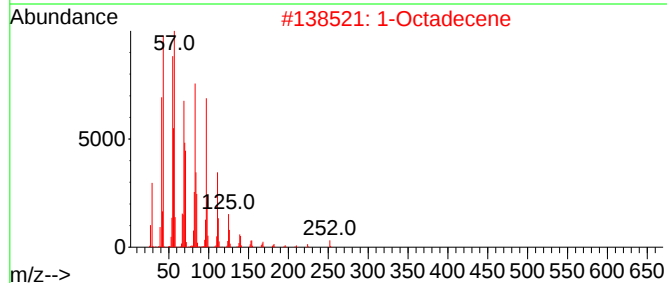
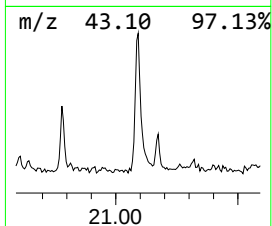
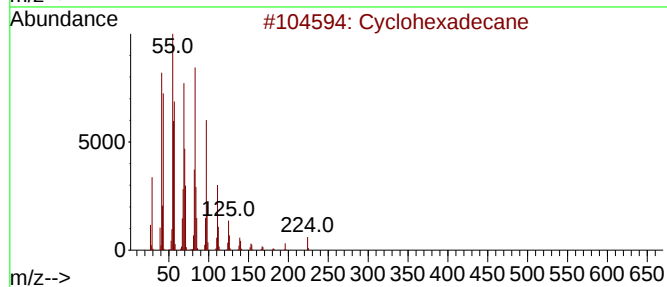
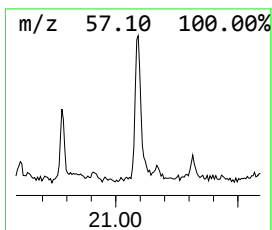
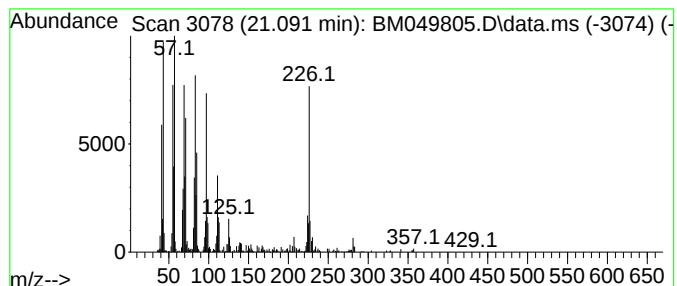
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.92 ng	588557	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			1-Octadecene	252	C18H36	000112-88-9	91
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	89
5			1-Hexacosanol	382	C26H54O	000506-52-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049805.D
Acq On : 03 Apr 2025 14:37
Operator : RC/JU
Sample : Q1693-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WCS-TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Glycolaldehyde ...	3.016	2.1	ng	175659	1	7.786	1647610	20.0
2-Pentanone, 4-...	4.904	16.7	ng	1377220	1	7.786	1647610	20.0
2-Pentanone, 4-...	5.981	2.9	ng	236797	1	7.786	1647610	20.0
Benzophenone	15.786	5.7	ng	763307	3	14.427	2700940	20.0
n-Hexadecanoic ...	18.074	5.7	ng	872865	4	17.168	3049330	20.0
Cyclohexadecane	21.092	2.9	ng	588557	5	21.403	4027320	20.0